

Exact realization of $SO(5)$ symmetry in extended Hubbard models

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Zhang recently conjectured an approximate $SO(5)$ symmetry relating antiferromagnetic and superconducting states in high- T_c cuprates. Here, an exact $SO(5)$ symmetry is implemented in a generalized Hubbard model (with long-range interactions) on a lattice. The possible relation to a more realistic extended Hubbard Hamiltonian is discussed.

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S.-C. Zhang recently conjectured that high- T_c cuprate compounds possess an approximate $SO(5)$ symmetry. [1]. His theory aims to explain the proximity of superconducting (SC) and antiferromagnetic (AF) phases in the phase diagram, and to account for the low-energy excitations as approximate $SO(5)$ Goldstone modes. Antiferromagnetism and superconductivity are unified in one grand order parameter field ($m^x, m^y, m^z, \text{Re}\Psi, \text{Im}\Psi$), behaving as a 5-component vector, where the first three elements are Cartesian components of the staggered magnetization and Ψ is a spin-singlet SC order parameter (Here “ $\text{Re}\Psi$ ” $\equiv \frac{1}{2}(\Psi + \Psi^\dagger)$, etc.)

In this picture, small symmetry-breaking terms tend to drive the system in a “superspin flop” between antiferromagnetism and superconductivity, just as, in a magnet with approximate $SO(3)$ symmetry, competing spin-space anisotropies and external field can drive a “spin-flop” transition between magnetic states with order along the z axis and in the xy plane. [1]

The $SO(5)$ theory, while positing an intimate relationship between SC and AF order, does not imply that the pairing mechanism is AF fluctuations [8,9]. Rather, it quantifies the notion (also relevant to superfluid ${}^3\text{He}$) that there need not be a sharp difference between interactions mediated by magnetic and “charge” (number) fluctuations. I pass over Zhang’s specific mechanism (whereby the system accommodates doping by switching from the AF state to a symmetry-related SC state which has a different particle number), for $SO(5)$ symmetry can be valid even if another sort of perturbation is found responsible for the symmetry breaking and the AF-SC transition.

The 41meV mode observed in spin-flip neutron scattering on $\text{YBa}_2\text{Cu}_3\text{O}_7$ [3] is interpreted as a Goldstone mode of $SO(5)$ with a gap due to the symmetry-violating terms, analogous to the anisotropy gap in a spin-wave branch of the uniaxial magnet [1]. These excitations are created by “ $\hat{\pi}^\dagger$ ” operators [4] ($SO(5)$ generators that mix magnetic and SC components). [5] They are charged bosons with the quantum numbers of “preformed” Cooper pairs, and presumably carry the current in the “normal” metal [1]; it has been speculated [7] that this explains the linear temperature dependence of the normal-state resistivity.

To the extent that $SO(5)$ -violating terms are small (as in Zhang’s phase diagram “A” [1]), relations between

AF and SC quantities are obviously predicted. For example, the Néel temperature T_N on one side ought to equal the SC T_c on the other side (the real ratio is 5 : 1 in $\text{YBa}_2\text{Cu}_3\text{O}_7$). Furthermore, when converted into the proper units, the tensors of superfluid density and AF spin stiffness should be equal; as should the order-parameter lengths (staggered moment and SC gap magnitude, respectively), and the interlayer couplings (interlayer superexchange and intrinsic Josephson coupling, respectively.) An order-of-magnitude equality of the interlayer couplings is indeed expected in the interlayer tunneling picture [10] Finally, the $SO(5)$ Ginzburg-Landau theory predicts that vortices have magnetic cores [1,11]; conversely, in analogy to the Bloch wall in the $SO(3)$ magnet, it suggests that magnetic domain walls contain SC stripes, as proposed for other reasons by Emery and Kivelson [12].

Microscopic $SO(5)$ symmetry — In this paper, using elementary notations, I implement a literal $SO(5)$ symmetry in a one-band lattice model, construct a Hamiltonian with exact $SO(5)$ symmetry, and finally consider whether a realistic Hamiltonian of an extended Hubbard form might approximate an $SO(5)$ symmetric Hamiltonian. Take a lattice with N sites (using periodic boundary conditions). Creation operators for the orbitals on site \mathbf{x} are $c_\sigma^\dagger(\mathbf{x})$ for $\sigma = \uparrow, \downarrow$. Let \mathbf{Q} be the ordering wavevector of some two-sublattice AF state, so that $e^{i\mathbf{Q}\cdot\mathbf{x}} = \pm 1$ at every site. The usual staggered-magnetization components are

$$\begin{aligned} m_z^{(c)}(\mathbf{x}) &\equiv \frac{1}{2}e^{i\mathbf{Q}\cdot\mathbf{x}}(c_\uparrow^\dagger(\mathbf{x})c_\uparrow(\mathbf{x}) - c_\downarrow^\dagger(\mathbf{x})c_\downarrow(\mathbf{x})), \\ m_+^{(c)}(\mathbf{x}) &\equiv e^{i\mathbf{Q}\cdot\mathbf{x}}(c_\uparrow^\dagger(\mathbf{x})c_\downarrow(\mathbf{x})) \end{aligned} \quad (1)$$

and $m_-^{(c)}(\mathbf{x}) \equiv m_+^{(c)}(\mathbf{x})^\dagger$. The SC order parameter operator has the general form $\Psi(\mathbf{x}) \equiv \sum_{\mathbf{r}, \mathbf{r}'} \psi(\mathbf{r}, \mathbf{r}') c_\downarrow(\mathbf{x} + \mathbf{r}) c_\uparrow(\mathbf{x} + \mathbf{r}')$ (which allows different spatial symmetries depending on the form of the coefficients $\psi(\mathbf{r}, \mathbf{r}')$.) We seek a continuous, unitary operation that turns a component of $\mathbf{m}(\mathbf{x})$ into one of $\Psi(\mathbf{x})$, i.e. turns creation into annihilation operators: clearly it must be some form of Bogoliubov transformation.

Indeed, a *discrete* $SO(3)$ symmetry of this sort is already known for the negative- U Hubbard model [13], for which the appropriate SC order parameter is $\Psi(\mathbf{x}) =$

$c_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})$. One maps $c_\downarrow(\mathbf{x}) \rightarrow e^{i\mathbf{Q}\cdot\mathbf{x}}c_\downarrow(\mathbf{x})^\dagger$ (leaving $c_\uparrow(\mathbf{x})$ alone) which implies $(\Psi(\mathbf{x})^\dagger, \Psi(\mathbf{x}), e^{i\mathbf{Q}\cdot\mathbf{x}}n(\mathbf{x})) \rightarrow (m_+(\mathbf{x}), m_-(\mathbf{x}), m_z(\mathbf{x}))$; here $n(\mathbf{x}) \equiv c_\uparrow^\dagger(\mathbf{x})c_\uparrow(\mathbf{x}) + c_\downarrow^\dagger(\mathbf{x})c_\downarrow(\mathbf{x})$. The only change induced in the Hubbard Hamiltonian is $U \rightarrow -U$; thus a hidden $SO(3)$ symmetry relates SC order (Ψ) and charge-density-wave order ($e^{i\mathbf{Q}\cdot\mathbf{x}}n(\mathbf{x})$) in the limit of large negative U .

To write the exact $SO(5)$ symmetry transparently, and to ensure it in the order parameters and Hamiltonians, I use the duality [16] between the “ c ” operators and an alternate set of canonically commuting operators,

$$d_{\mathbf{k}+\mathbf{Q},\sigma} \equiv \eta_{\mathbf{k}}c_{\mathbf{k}\sigma} \quad (2)$$

In real space, this says

$$d_\sigma(\mathbf{x}) = e^{-i\mathbf{Q}\cdot\mathbf{x}} \sum_{\mathbf{r}} \varphi(\mathbf{r})c_\sigma(\mathbf{x} + \mathbf{r}) \quad (3)$$

where $\eta_{\mathbf{k}} \equiv \sum_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}\varphi(\mathbf{r})$. To make the symmetry (5b) work, we will need the important conditions [15]

$$\eta_{\mathbf{k}+\mathbf{Q}} = -\eta_{\mathbf{k}} \quad (4a)$$

$$\eta_{-\mathbf{k}} = \eta_{\mathbf{k}} \quad (4b)$$

for all \mathbf{k} , which in real space say respectively that $\varphi(\mathbf{r}) = 0$ for “even” \mathbf{r} (meaning those connecting sites in the same sublattice) and that $\varphi(\mathbf{r}) = \varphi(-\mathbf{r})$. Eq. (4a) implies $\{c_\sigma^\dagger(\mathbf{x}), d_{\sigma'}(\mathbf{x}')\} = 0$ if \mathbf{x} and \mathbf{x}' are on the same sublattice (e.g. $\mathbf{x} = \mathbf{x}'$). [14] Then the symmetry operation is just

$$c'_\sigma(\mathbf{x}) = \cos(\phi/2)c_\sigma(\mathbf{x}) + \sin(\phi/2)d_{-\sigma}^\dagger(\mathbf{x}) \quad (5a)$$

$$d'_\sigma(\mathbf{x}) = -\sin(\phi/2)c_{-\sigma}^\dagger(\mathbf{x}) + \cos(\phi/2)d_\sigma(\mathbf{x}) \quad (5b)$$

The symmetry (5b) is generated by $\frac{1}{2}(\hat{\pi} + \hat{\pi}^\dagger)$, where $\hat{\pi} = i \sum_{\mathbf{x}} [c_\downarrow(\mathbf{x})d_\uparrow(\mathbf{x}) - d_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})]$. To transform wavefunctions, it is useful to know that the vacuum $|0\rangle$ transforms to $\prod_{\mathbf{k}} (\cos(\phi/2) + \eta_{\mathbf{k}} \sin(\phi/2)c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}+\mathbf{Q},\downarrow}^\dagger)|0\rangle$.

So that it will map exactly under (5b), the $SO(5)$ staggered magnetization must be defined as

$$\mathbf{m}(\mathbf{x}) = \frac{1}{2}[\mathbf{m}^{(c)}(\mathbf{x}) - \mathbf{m}^{(d)}(\mathbf{x})] \quad (6)$$

where $\mathbf{m}^{(d)}$ is (1) with “ c ” → “ d ”. Note this gives a sensible result for the Néel state: if $\mathbf{m}^{(c)}(\mathbf{x})$ is up, then $\mathbf{m}^{(d)}(\mathbf{x})$ is down (since the d “orbital” on site \mathbf{x} is a linear combination of “ c ” orbitals from the opposite sublattice).

The SC order parameter is

$$\Psi(\mathbf{x}) \equiv e^{i\mathbf{Q}\cdot\mathbf{x}} \frac{1}{2}[c_\downarrow(\mathbf{x})d_\uparrow(\mathbf{x}) + d_\downarrow(\mathbf{x})c_\uparrow(\mathbf{x})] \quad (7)$$

Then

$$m_z'(\mathbf{x}) = \cos\phi m_z(\mathbf{x}) + \sin\phi \operatorname{Re}\Psi(\mathbf{x}) \quad (8a)$$

$$\operatorname{Re}\Psi'(\mathbf{x}) = \cos\phi \operatorname{Re}\Psi(\mathbf{x}) - \sin\phi m_z(\mathbf{x}) \quad (8b)$$

while the other three components are invariant. The $SO(5)$ rotation of the Néel state with $\phi = \pi/2$ gives

$$2^{-N/2} \prod_{\mathbf{k}} (1 + \eta_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle \quad (9)$$

This BCS state has no remnant of Fermi surface ($\langle c_\sigma^\dagger c_\sigma \rangle \equiv 1/2$ throughout reciprocal space.)

One could construct a total of six such rotations, each of which mixes one of the three components of $\mathbf{m}(\mathbf{x})$ with one of the two components of $\Psi(\mathbf{x})$. The other five could all be obtained by combining (5b) with the usual $SO(3)$ rotations acting on the spin labels of c and d operators, plus the usual $SO(2) \equiv U(1)$ gauge symmetry changing their complex phases. (Zhang has discussed the algebra of $SO(5)$ generators [1,2].)

For the square lattice, we must have $\mathbf{Q} = (\pi, \pi)$ so the hopping term (12) will be $SO(5)$ -invariant. This leaves much freedom to $\eta_{\mathbf{k}}$, but the simplest choice is

$$\eta_{\mathbf{k}} \equiv \operatorname{sign}(\cos k_x - \cos k_y) \quad (10)$$

This is inspired by the original and approximate $SO(5)$ symmetry [1] which had the same form but with coefficients $\eta_{\mathbf{k}} \rightarrow \cos k_x - \cos k_y$; recently Kohno [2] independently discovered the exact version (10). Comparison with (9) shows that (10) is essentially the Cooper pair wavefunction and has $d_{x^2-y^2}$ pairing symmetry, consistent with strong experimental evidence in the cuprates [17]. Interestingly, one other simple form would also satisfy the conditions (4): $\eta_{\mathbf{k}} \equiv \operatorname{sign}(\cos k_x + \cos k_y)$. That variant of $SO(5)$, which entails “extended s -wave” pairing, appears free from internal contradictions (contrary to a suggestion in Ref. [1]).

The coefficients in (3) (Fourier transform of (10)) are $\varphi(x, y) = 4/[\pi^2(x^2 - y^2)]$ for $x + y$ odd, zero for $x + y$ even. For numerical and analytic explorations, it may also be helpful to have a one-dimensional toy realization of $SO(5)$ symmetry. This is given by $Q = \pi$ and $\eta_{\mathbf{k}} \equiv \operatorname{sign}(\cos k)$, which gives $\varphi(r) = 2(-1)^{(r-1)/2}/(\pi r)$ for r odd, zero for r even.

Microscopic Hamiltonian — Next I will produce an artificial generalization of the Hubbard Hamiltonian which has exact $SO(5)$ symmetry. The basic Hubbard model with particle/hole symmetry can be written

$$\mathcal{H}_{Hubb} = \mathcal{H}_{hop} + U \sum_{\mathbf{x}} \frac{1}{2}(n(\mathbf{x}) - 1)^2, \quad (11)$$

$$\mathcal{H}_{hop} = (-t) \sum_{\mathbf{x}\sigma} \sum_{\mathbf{u}} c_\sigma^\dagger(\mathbf{x})c_\sigma(\mathbf{x} + \mathbf{u}) = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad (12)$$

with \mathbf{u} running over nearest neighbors, and $\epsilon_{\mathbf{k}} = (-t)(\cos k_x + \cos k_y)$.

The minimal Hamiltonian including the terms in (11) is simply the $SO(5)$ symmetrization of (11). The hopping term \mathcal{H}_{hop} is already invariant under all the $SO(5)$ rotations (such as (8b)), provided that $\epsilon_{\mathbf{k}+\mathbf{Q}} = -\epsilon_{\mathbf{k}}$. That

is true in any bipartite lattice, if and only if \mathbf{Q} describes the original Néel state with opposite spins orientations on nearest-neighbor sites.

However, $SO(5)$ symmetrization turns the number operator $n(\mathbf{x})$ to something quite different, $n^s(\mathbf{x}) \equiv \frac{1}{2}[n(\mathbf{x}) - n^{(d)}(\mathbf{x})]$. (I take the obvious definition $n^{(d)}(\mathbf{x}) \equiv d_{\downarrow}^\dagger(\mathbf{x})d_{\downarrow}(\mathbf{x}) + d_{\uparrow}^\dagger(\mathbf{x})d_{\uparrow}(\mathbf{x})$.) In contrast to the usual number operator, $\sum_{\mathbf{x}} n^s(\mathbf{x}) \equiv 0$. The $n^{(d)}(\mathbf{x})$ operator includes terms $|\varphi(\mathbf{r})|^2 n(\mathbf{x} + \mathbf{r})$, all on the opposite sublattice from \mathbf{x} and largest for nearest neighbors, $|\mathbf{r}| = 1$, as well as long range hopping between sites of the same sublattice. Thus the $SO(5)$ -symmetrized Hubbard model has a modified interaction term:

$$\mathcal{H}^s = \mathcal{H}_{hop} + U^s \sum_{\mathbf{x}} (n^s(\mathbf{x}))^2 \quad (13)$$

When we expand $n^s(\mathbf{x})^2$, we get a variety of terms, which include interactions and hoppings (with diminishing coefficients) to arbitrarily large distances.

What is the ground state of (13)? If $U^s \rightarrow 0$, at half-filling, it is the Fermi sea which manifestly possesses $SO(5)$ symmetry. The $t \rightarrow 0$ limit of (13) is more relevant and more challenging. Certainly a ground state is obtained at half filling by setting the even sublattice ferromagnetic in one direction and the odd sublattice ferromagnetic in any another direction, since $n(\mathbf{x}) = n^{(d)}(\mathbf{x}) = 1$ on every site. The two sublattice moments can be added to make a total angular momentum l taking any value $\{0, 1, \dots, N\}$. As was pointed out by Ref. [2], by applying the $\hat{\pi}$ and $\hat{\pi}^\dagger$ operators, as well as familiar spin-space rotations, each angular momentum is part of an $SO(5)$ multiplet with a total degeneracy [19] $(l+1)(l+2)(2l+3)/6$. This includes states with particle numbers differing from N by multiples of ± 2 . The total degeneracy of this family of states is thus $(N+1)(N+2)^2(N+3)/12$, small compared to 2^N in the ordinary Hubbard model (11) with $t = 0$; however, conceivably this family does not exhaust the ground states.

Now consider how a small t value splits these states in second-order perturbation theory. Among the states in which each sublattice is ferromagnetic aligned, this will have exactly the same effect as it does in the Hubbard model. This suggests that the Néel state in fact approximates one of the ground states – and so must (9), the $SO(5)$ rotation of the Néel state, since \mathcal{H} has $SO(5)$ symmetry: thus I conjecture the $t \ll U^s$ ground state has $SO(5)$ broken symmetry.

Group theory could be used to enumerate additional allowed terms in the Hamiltonian as in [2]; in particular, a bilinear coupling of the order parameter on neighboring sites ($SO(5)$ symmetrization of the exchange interaction). However, I have avoided this $SO(5)$ t - J model analog. It could be derived (in the fashion I just outlined, with $|J| \sim t^2/U^s$) from the $SO(5)$ Hubbard-model analog in the $t \ll U^s$ limit. But the most interesting

phases of the standard t - J model occur in the regime of large J/t , which cannot be derived from any regime of the Hubbard model [9], and the same thing may happen for the $SO(5)$ -Hubbard model (13).

Comparison to an extended Hubbard model — I now discuss how one might search for approximate $SO(5)$ symmetry in some Hubbard-like model, such as

$$\mathcal{H}_{ext} = \mathcal{H}_{Hubb} + \mathcal{H}'_{hop} + \frac{1}{2}V \sum_{\mathbf{xu}} n(\mathbf{x})n(\mathbf{x} + \mathbf{u}) \quad (14)$$

In (14) \mathcal{H}'_{hop} has the form of (12), except that the coefficient is t' and the displacement is \mathbf{u}' running over *second* neighbors. The last term in (14) is a Coulomb repulsion between nearest neighbor sites. Comparison of measurements and calculations of electronic structure [22] suggest that $U/t \geq 4$ and perhaps $t'/t \approx -0.3$ in cuprates. The aim is to find the point(s) in the parameter space of \mathcal{H}_{ext} which make it closest to (13): can the parameters U , V , and t' of (14) be related to U^s in (13)?

We can very crudely guess at the U terms simply by retaining only the terms from (13) of exactly this form. They come not only from $n(\mathbf{x})^2$ but also from expanding of $n^{(d)}(\mathbf{x})^2$. The result is $U = \frac{1}{4}U^s(1 + \sum_{\mathbf{r}} |\varphi(\mathbf{r})|^4) = \frac{1}{4}U^s(1 + 1/9)$.

We can estimate V in the same fashion, from the nearest-neighbor term in $n(\mathbf{x})n^{(d)}(\mathbf{x})$ obtaining $V = -U^s|\varphi(\mathbf{u})|^2$ where \mathbf{u} is a nearest neighbor. Here the $SO(5)$ symmetry demands an *attractive* nearest-neighbor electron interaction, which is understandable: in the $U^s \rightarrow \infty$ limit, only singly-occupied states can occur in a ground state, so only the AF states could be ground states. The SC state has a certain density of doubly-occupied and vacant sites, so an additional term is needed to equalize its energy with that of the AF state. Any pairing interaction might play the same role.

Finally, no t' terms appear in (13). In fact, any single-electron hopping term within the same sublattice violates $SO(5)$ symmetry and gets annihilated in the $SO(5)$ symmetrization. Thus, although there are many *quartic* terms in (13) that do hop electrons between sites on the same sublattice, there is no $SO(5)$ symmetric way of decoupling these terms to generate \mathcal{H}'_{hop} . (But in second-order perturbation theory, those quartic terms can generate e.g. second-neighbor exchange interactions, just as the t' terms can.)

Very recently, an extended Hubbard model has been diagonalized using a new interaction with double hoppings, [18] $\sum_{\mathbf{x}} K(\mathbf{x})^2$, where $K(\mathbf{x}) = \sum_{\sigma\mathbf{u}} c_{\sigma}^\dagger(\mathbf{x})c_{\sigma}(\mathbf{x} + \mathbf{u}) + c.c.$. That is closer to (13), since its terms have the same form as the largest terms (after those already mentioned) in $n(\mathbf{x})n^d(\mathbf{x})$ and $(n^d(\mathbf{x}))^2$. This model has an apparently continuous AF/SC transition, [18] so it may well realize $SO(5)$ approximately.

Of course, even at the $SO(5)$ multicritical point in Zhang's picture, the *microscopic* Hamiltonian might have

no visible $SO(5)$ symmetry; just as at the “spin-flop” point of an anisotropic magnet, a cancellation of terms favoring competing kinds of order might suffice, with the symmetry emerging only at long-wavelengths [1]. But if that length scale is much larger than the numerically tractable system size for Hubbard models, then direct numerical calculations on finite lattices (such as [20]) are too small to address the order parameter symmetry.

Exact diagonalizations (e.g. [20]) commonly study ground-state correlations, but their spatial decay is often inconclusive as a test of order due to small system size. Yet it is possible that the (excited) eigenstates show a well-defined structure characteristic of a particular symmetry; this provided the convincing evidence for long-range order in the spin-1/2 triangular lattice AF [21]. (Very recently, Ref. [19] has pursued exactly such a program in exact diagonalizations of the t - J model). I suggest identifying an $SO(5)$ multiplet numerically in a model with manifest $SO(5)$ symmetry, [19] and then following its evolution while the Hamiltonian is adiabatically modified to a more realistic model such as (14).

Conclusion — I have identified inklings of $SO(5)$ symmetry in popular existing models and exhibited the form an exact $SO(5)$ symmetry could take in one- or two-dimensional lattice models. The $SO(5)$ symmetry in microscopic models is promising as a spur to the comparison or unification of competing models of high- T_c superconductivity, and to improved understanding of extended Hubbard models. However, I have not addressed the murkier issue of its application to the cuprates.

Of the objections mounted so far to a possible $SO(5)$ relationship between the actual AF and SC phases, one seems to be really inescapable: the Fermi surface [6]. If the SC metal shows a sharp drop in electron occupation along a certain surface in reciprocal space, as found in angle-resolved photoemission experiments [25], then (see (2)) its AF image under $SO(5)$ has a similar surface (shifted by \mathbf{Q}). Apparently this AFM must be a spin-density-wave metal [24]. But the real AF phase of the cuprates is instead deemed to be a Mott insulator [9], and its AF correlations are well modeled using a nearest neighbor exchange Hamiltonian [23].

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